

CONSTITUTIVE MODELING OF SUPERALLOY SINGLE CRYSTALS
WITH VERIFICATION TESTING*Eric Jordan
University of ConnecticutKevin P. Walker
Engineering Science Software, Inc.

INTRODUCTION

The prediction of component life is an important activity in the development of gas turbine engines. Such predictions require accurate component stress analysis. In cases involving inelastic strain at elevated temperatures these analyses are performed numerically and use constitutive equations as an essential part of the analysis. The goal of the research described in this paper is the development of constitutive equations to describe the elevated temperature stress-strain behavior of single crystal turbine blade alloys. The program involves both the development of a suitable model and verification of the model through elevated temperature tension-torsion testing. A constitutive model is derived from postulated constitutive behavior on individual crystallographic slip systems. The behavior of the the entire single crystal is then arrived at by summing up the slip on all the operative crystallographic slip systems. This type of formulation has a number of important advantages, including the prediction of orientation dependence and the ability to directly represent the constitutive behavior in terms which metallurgists use in describing the micromechanisms. Along with the model development is a biaxial test program that will generate data to determine the model constants, provide insight into the qualitative aspects of the material behavior and provide data to verify the usefulness of the constitutive model. In the remainder of the report the model will be briefly described followed by the experimental set-up and some of the experimental findings to date. Finally, several simulations of the experimental data using the model will be presented.

BASIC MODEL FORMULATION

The inelastic anisotropic behavior of the single crystal superalloy is derived from a crystallographic slip model. In nickel-base superalloy single crystals crystallographic slip occurs on both the octahedral and cube planes, and it is necessary to incorporate both of these slip systems in the model. Indeed, as will be discussed in the simulation section, the anisotropic constitutive behavior of single crystal superalloys such as PWA 1480 cannot be modelled using only the octahedral slip system.

The constitutive behavior is assumed to be governed by the following set of equations:

* Work done under NASA Grant NAG3-512.

$$\sigma_{ij} = Q_{ji} Q_{kl} D_{jkmn} (\varepsilon_{mn} - \varepsilon_{mn}^P),$$

where Q_{ij} is the matrix of direction cosines between the global and crystallographic axes, and the inelastic strain rate is given by the expression:

$$\dot{\varepsilon}_{ij}^P = \sum_{r=1}^{12} (\dot{\gamma}_r/2) [(i, \underline{n}_r^0)(\underline{m}_r^0, j) + (i, \underline{m}_r^0)(\underline{n}_r^0, j)] + \sum_{r=1}^6 (\dot{\xi}_r/2) [(i, \underline{n}_r^c)(\underline{m}_r^c, j) + (i, \underline{m}_r^c)(\underline{n}_r^c, j)],$$

and

$$\dot{\gamma}_r = K_r^{-p} (\pi_r - \omega_r) |\pi_r - \omega_r|^{p-1}, \quad \dot{\xi}_r = L_r^{-t} (\tau_r - \Omega_r) |\tau_r - \Omega_r|^{t-1},$$

$$\dot{\omega}_r = \rho_1 \dot{\gamma}_r - \rho_2 |\dot{\gamma}_r| \omega_r - \rho_3 |\omega_r|^{m-1} \omega_r, \quad \dot{\Omega}_r = \rho_6 \dot{\xi}_r - \rho_7 |\dot{\xi}_r| \Omega_r - \rho_8 |\Omega_r|^{n-1} \Omega_r,$$

$$\dot{K}_r = \left\{ \sum_{k=1}^{12} [h_{rk} - \eta_1 \{K_r - K_r^1\}] |\dot{\gamma}_k| \right\} - h_1 \{K_r - K_r^1\}^s,$$

$$\dot{L}_r = \left\{ \sum_{k=1}^6 [\beta_2 - \eta_2 \{L_r - L_r^0\}] |\dot{\xi}_k| \right\} - h_2 \{L_r - L_r^0\}^u,$$

$$h_{rk} = \beta_1 \{q + (1-q)\delta_{rk}\}, \quad K_r^1 = K_r^0 + \rho_4 \kappa_r + \rho_5 |\varphi_r|,$$

where π_r and τ_r are the resolved shear stress components on the octahedral and cube planes, respectively, whilst κ_r represents the resolved shear stress component in the $\langle 112 \rangle$ direction on the octahedral plane and produces a yield stress asymmetry. The term φ_r is the resolved shear stress on the cube plane in the direction of the octahedral slip direction and this term is also involved in the yield stress asymmetry. The terms ω_r and Ω_r represent the back stress components on the octahedral and cube planes, and K_r and L_r are the corresponding drag stress state variables. The constant, q , in the expression for the drag stress evolution equation allows for latent hardening in the single crystal slip systems. At 871C, no latent hardening has been detected, and we have accordingly set $q=1$.

The material constants for the simulations were taken to have the following values:

$$\rho_1 = 4.509 \times 10^7, \quad \rho_2 = 645, \quad \rho_3 = 9.8 \times 10^{-6}, \quad \rho_4 = 0, \quad \rho_5 = 0, \quad K_r^0 = 25775, \quad m = 1.49, \quad p = 6.69, \quad s = 1, \\ \beta_1 = 0, \quad \eta_1 = 0, \quad q = 1, \quad \rho_6 = 1.506 \times 10^7, \quad \rho_7 = 1000, \quad \rho_8 = 9.7 \times 10^5, \quad L_r^0 = 71152, \quad n = 1.05, \quad t = 7.09, \\ \beta_2 = 0, \quad \eta_2 = 0, \quad h_2 = 0, \quad u = 0, \quad D_{1111} = 31.37 \times 10^6, \quad D_{1122} = 20.84 \times 10^6, \quad D_{1212} = 21.26 \times 10^6.$$

The foregoing material constants were determined with the COPES-CONMIN general purpose optimization code, which used about one hour of computer time on an IBM PC-XT with an 8087 math coprocessor chip. This speed is due to the fact that simplified formulae are available for the inelastic strain rate in the $\langle 001 \rangle$

direction for octahedral and cube slip.

As shown in the simulations it is necessary to include both octahedral and cube slip in the theoretical formulation in order to capture the tension-torsion biaxial behavior of single crystal superalloys such as PWA 1480.

EXPERIMENTS AND RESULTS

The determination of model constants and model verification is being carried out using an elevated temperature (871C) tension-torsion servohydraulic test set-up developed as part of a fatigue research program (NASA NAG3-160). The maximum temperature capability of the system was increased during this program. The basic servohydraulic is a 2500 N-M , 250 KN servohydraulic tension-torsion machine differing from the commercial machines only by virtue of a University of Connecticut developed load frame made from a large die set. Force and torque are measured with a conventional strain gage load-torque cell while strain is measured by a University of Connecticut designed extensometer that utilizes high temperature noncontacting displacement probes. This extensometer, shown in Fig.1, allows testing in excess of 871C without any need to cool the extensometer. The machine is computer controlled using a DEC LSI-1123 microcomputer and software developed under this grant. The software allows a wide variety of tests to be run including tests involving a sudden change in strain rate, known (cf. reference (2)), to be useful in assessing the drag stress state variables used in the anisotropic constitutive model. The software also allows strain holds to be inserted into a strain history which is particularly useful in assessing the back stress variable (reference(3)). The material being tested is a high volume (65%) gamma-prime single crystal material, PWA 1480, graciously supplied by Pratt & Whitney.

The tests run are unique, being the first biaxial tension-torsion tests run on this type of single crystal alloy. Biaxial testing has the special advantage that orientation effects may be studied by varying the stress state as opposed to growing specimens in a wide variety of configurations as is usually done for uniaxial testing. Early experiments with this material show that at 871C (1600F) it is possible to return the material to the same deformation state by applying a few repeated cycles of almost any strain history. As a result a large number of different types of tests can be run on a single specimen. Some of the more interesting results will quickly be presented. Figure 2 shows strain rate dependence in torsion and it is qualitatively similar to tension results. When combined with tension tests these torsion results provide a powerful and easy way to determine the relative proportions of octahedral slip and cube slip, which is vital to the success of the proposed model. This will be elaborated in the next section. Many materials are known to cyclically harden to a much greater degree in non-proportional loading, reference (3), and it is important to determine if PWA 1480 exhibits this common behavior. A test series was run in which a torsional loop was taken followed by cycling with a torsion to tension strain ratio (λ) of 1.5 and with tension and torsion 90 degrees out-of-phase. This type of non-proportional cycling is known to be especially effective, reference (3), in producing extra hardening. Figure 3 shows the torsional loops before and after this cycling and the loops are so similar as to be nearly indistinguishable indicating that there is no extra hardening. Finally, these

alloys are known to exhibit tension-compression yield stress asymmetry which is predicted by the proposed model, reference (4). This asymmetry should also manifest itself in biaxial tests. Figure 4 shows the asymmetry as a function of the lambda ratio (λ). It is apparent that at 1600F there is little asymmetry except at the smallest lambda ratios. Because the torsion loops are very small at these lambda ratios. These findings will be rechecked in an additional experiment. If confirmed this data will provide a further test of the ability of the proposed model to predict asymmetry. Future testing will include other test temperatures and will examine the anisotropy of the back stress and drag stress through the use of two rate tests and biaxial strain hold tests.

SIMULATIONS USING THE MODEL

The tubular specimens are oriented with the cylindrical axes along the $\langle 001 \rangle$ crystallographic direction. When pulled in the axial direction the resolved shear stresses on the crystallographic cube planes are zero and only octahedral slip occurs. Material constants for the octahedral slip component of the constitutive model were most conveniently derived from the uniaxial data obtained at Pratt & Whitney. Figure 5 shows the experimental uniaxial data for PWA 1480 at 871C at strain rates of 10^{-3} , 10^{-4} and 10^{-5} per second in the $\langle 001 \rangle$ direction and Fig. 6 shows the corresponding loops predicted with the constitutive model which agree well with the data. A check was made to ensure that the Pratt & Whitney uniaxial data, obtained from a different heat of material and with a bar instead of a tubular specimen, was comparable to the data collected in this program. The loops generated at Pratt & Whitney and at the University of Connecticut at 0.8 percent strain range and a strain rate of 10^{-3} per second were practically indistinguishable. Thus, the material constants obtained from the test at Pratt & Whitney correctly predict the uniaxial data obtained at the University of Connecticut.

Figure 2 shows torsional hysteresis loops carried out at a strain rate of 10^{-3} , 10^{-4} and 5×10^{-5} per second at a strain range of 0.6%. If only octahedral slip is included in the constitutive model the predicted loops, shown in Fig 7, are too narrow. Inclusion of cube slip in the model widens the predicted torsional loops and the predictions with combined octahedral and cube slip are shown in Fig. 8. Comparison of the data in Fig. 2 and the prediction from the combined octahedral and cube slip theory in Fig. 8 shows very good agreement. It is worth noting that $\langle 001 \rangle$ tension data is especially suitable for the determination of the octahedral slip constitutive constants, since cube slip is inoperative for this direction under uniaxial loading conditions. Torsion tests will involve both cube slip, if operative, and octahedral slip and can be used to determine the cube slip constants once the octahedral constants have been determined from the $\langle 001 \rangle$ uniaxial data. Comparison of the predicted torsional loops, using octahedral slip only, can be used to detect the occurrence of cube slip which is usually found only by laborious slip trace studies that are very difficult to conduct at temperatures above 593C (1100F).

SUMMARY

A slip system based constitutive model has been formulated for PWA 1480

which represents explicitly both octahedral slip and cube slip. Tension-torsion tests on single crystal material have been run at 871C and some of the torsional results have been successfully simulated using the model. It was found that the prediction of torsion data from tension data was only successful if the correct combination of cube and octahedral slip was used. The prediction of torsion data is a useful tool in determining which slip modes are active. Future work will involve simulations of various biaxial test conditions and will also attempt to simulate tests with variable strain rates and strain holds. The results of the initial simulations are very encouraging and generation of more challenging test cases in the lab and the simulation of these more complex cases is expected to be an interesting exercise of the constitutive model development.

REFERENCES

1. Krempl, E., RPI Report No. RPI CS 78-5, 1978.
2. Oytana, H.S. and Sidebottom, O.M., "Constitutive Equations Study in Biaxial Stress Experiments," J. of Eng. Mat. and Tech., Trans. of ASME Ser. H, Vol. 104, Jan. 82, p. 1.
3. Lamba, H.S. and Sidebottom, O.M., "Cyclic Plasticity for Non-proportional Paths: Part I - Cyclic Hardening Experiments," J. of Eng. Mat. and Tech., Trans. of ASME Series H, Vol. 100, Jan. 78, p. 104.
4. Shah, D. and Lin, L., J. Metals, Vol. 32, No. 8, p. 62, 1980.

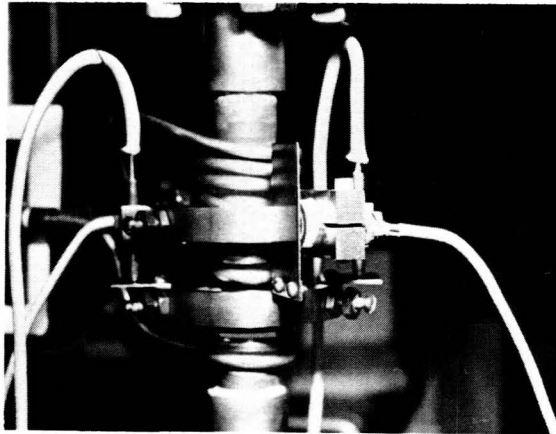


Figure 1: Single crystal specimen with extensometer and induction heater during biaxial test at 1600°F.

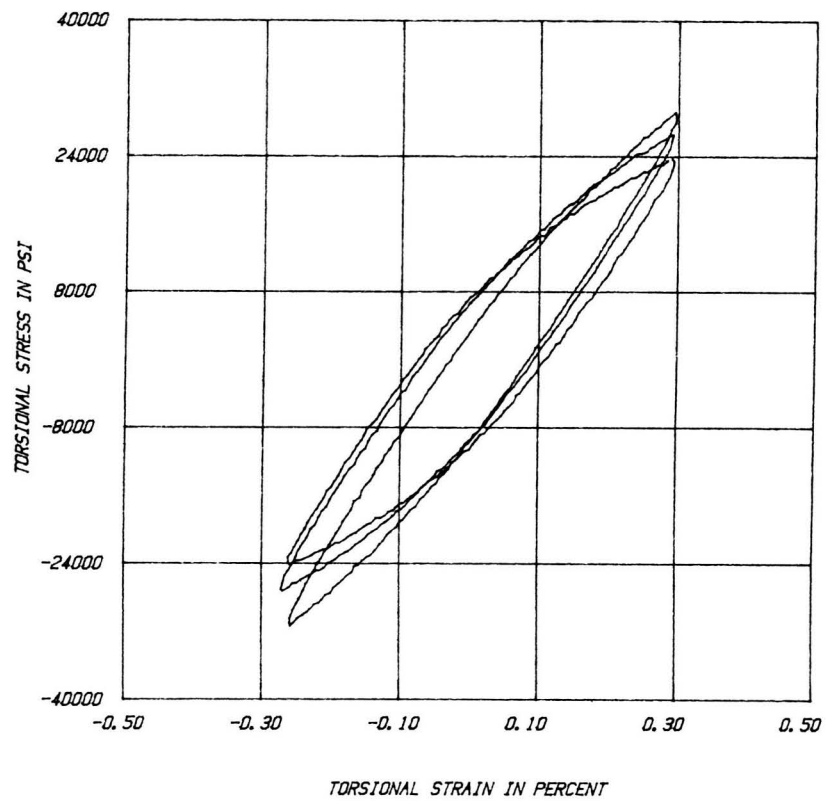


Figure 2: EXPERIMENTAL TORSIONAL LOOPS FOR PWA 1480 AT 1600°F

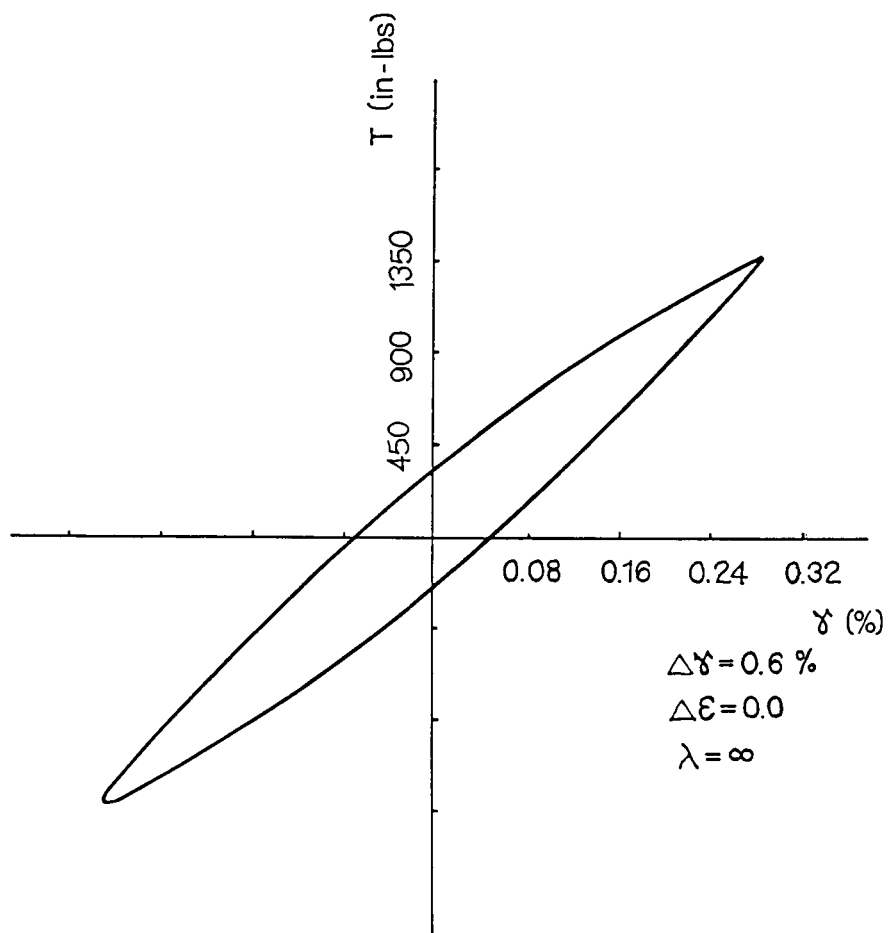
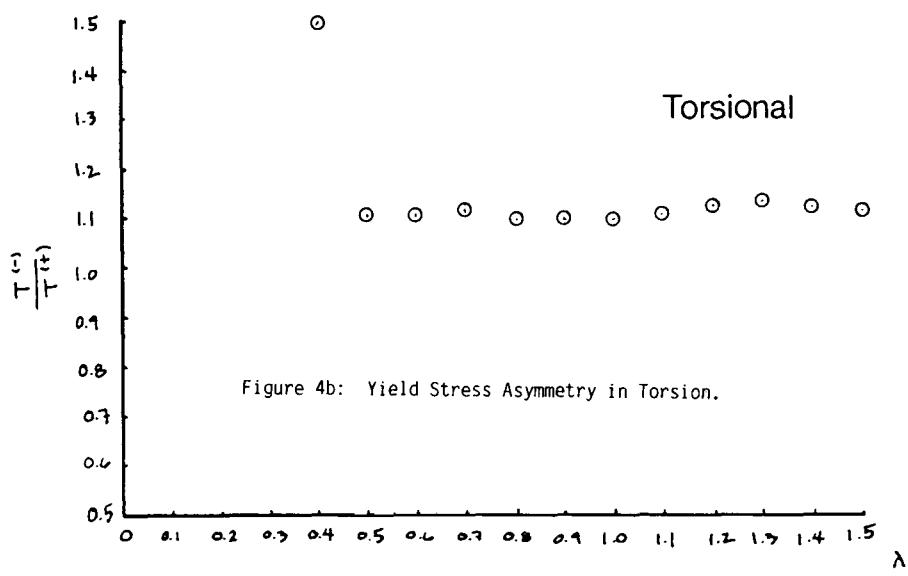
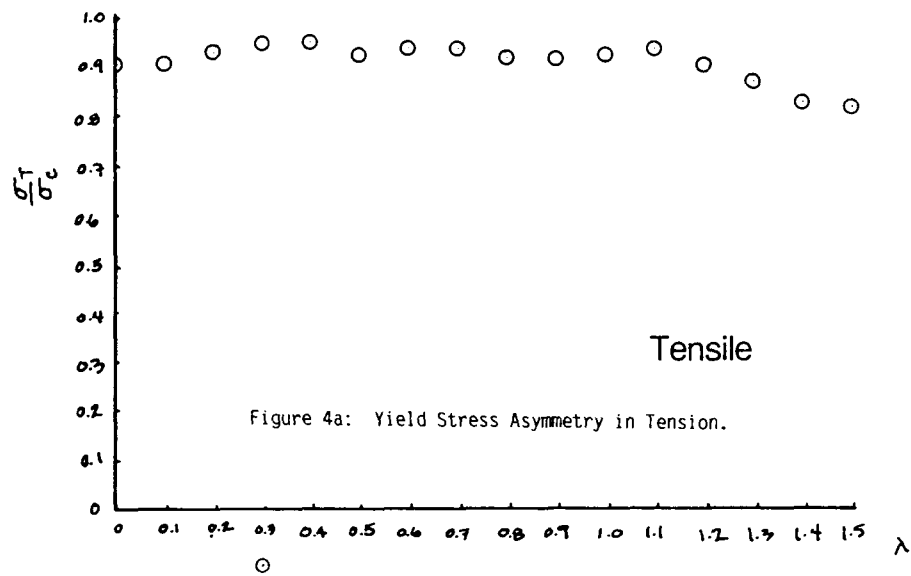


Figure 3: Torsional Loops Before and After Nonproportional Loading Cycles.

YIELD ASYMMETRY



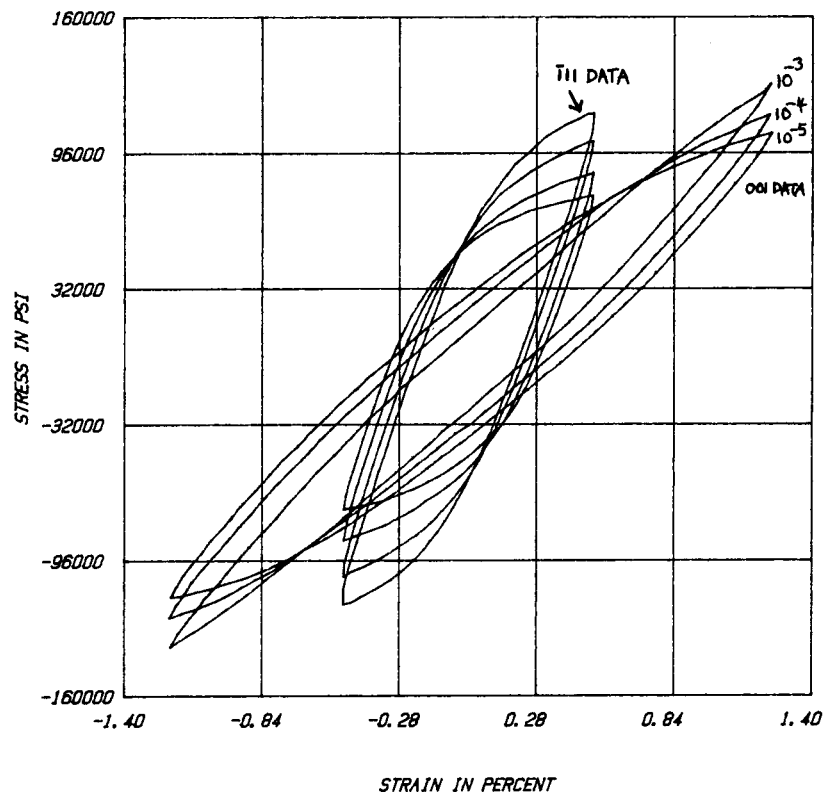


Figure 5: PWA 1480 EXPERIMENTAL HYSTERESIS LOOPS AT 1600F

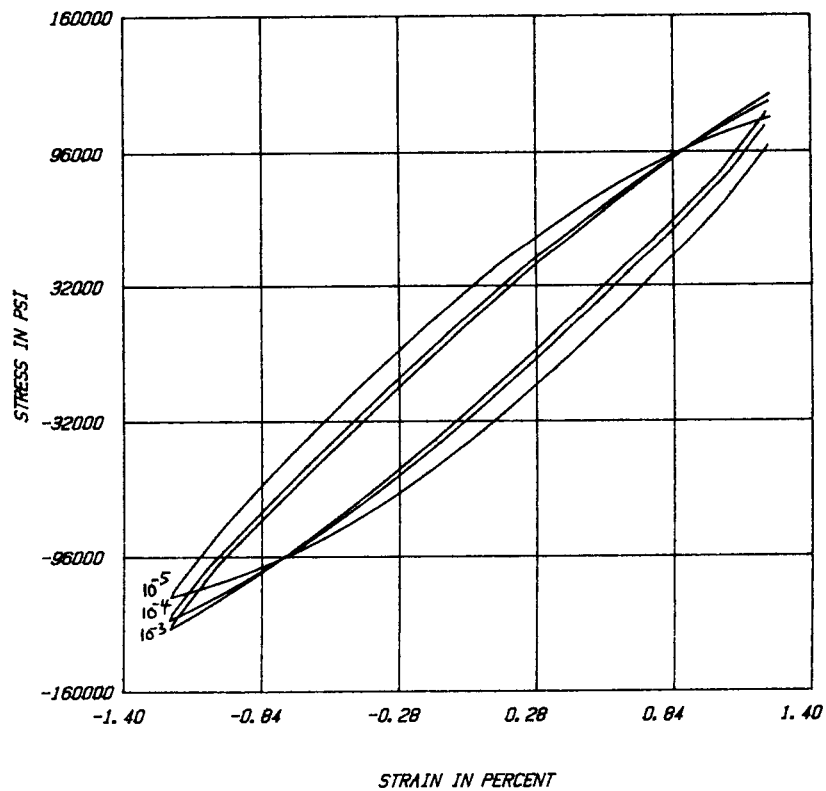


Figure 6: PREDICTED LOOPS FOR PWA 1480 AT 1600F (OOI DIRECTION)

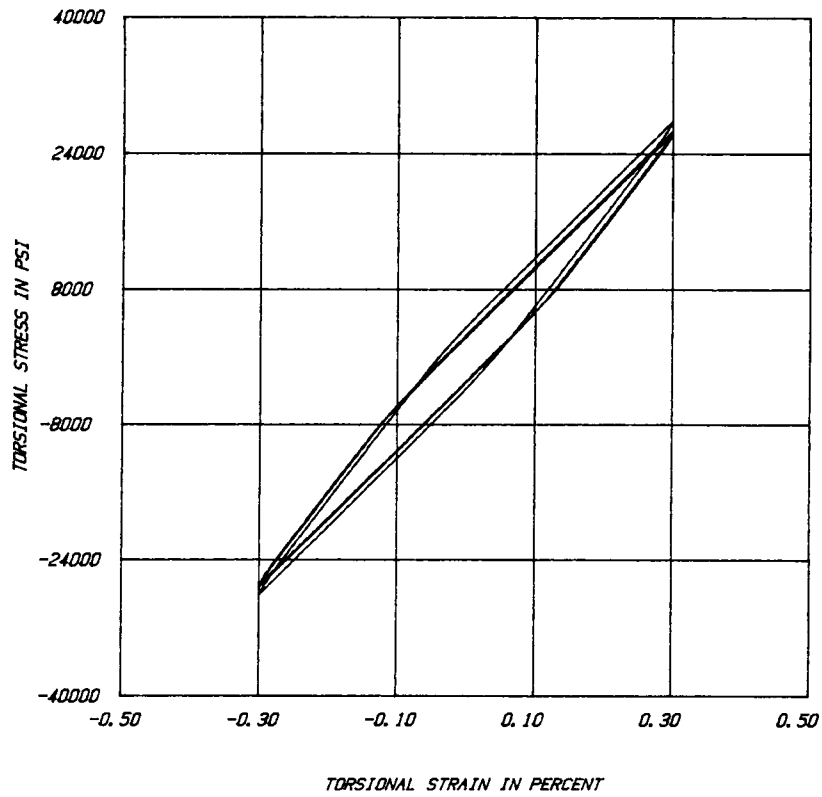


Figure 7: *PREDICTED TORSIONAL LOOPS WITH OCTAHEDRAL SLIP*

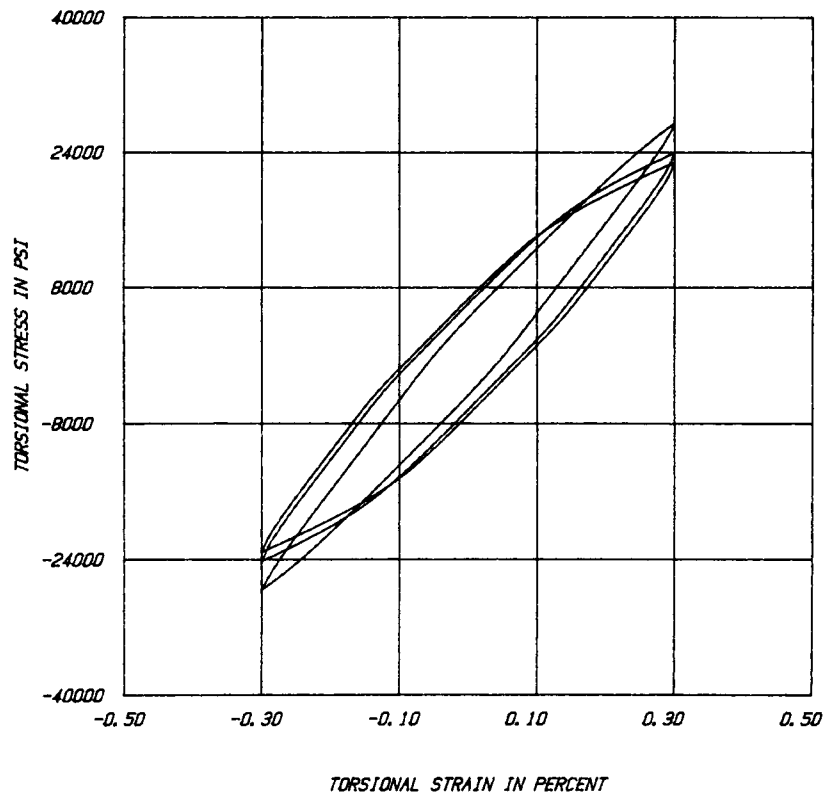


Figure 8: *PREDICTED TORSIONAL LOOPS WITH OCTAHEDRAL AND CUBE SLIP*